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TECHNIQUES FOR OPTIMIZING A QUADRUPOLE GC/MS/COMPUTER SYSTEM

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TECHNIQUES FOR OPTIMIZING A QUADRUPOLE GC/MS/COMPUTER SYSTEM

Environmental Research Laboratory
Office of Research and Development
U.S. Environmental Protection Agency
Athens, Georgia 30601

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SECTION I

CONCLUSIONS AND RECOMMENDATIONS

Appropriate operator techniques are essential in maintaining the sensitivity and stability of the Finnigan 1015 GC/MS/Computer system. The utility of the data acquired can be improved significantly by operator action.

The techniques discussed herein have been found to be effective on our system. Other users of this type instrumentation should employ these techniques when necessary.

SECTION II

INTRODUCTION

The most powerful tool currently in use for the analysis of organic pollutants is computerized Gas Chromatography/Mass Spectrometry. Since this instrumentation represents a sizable investment, it should be available for use as much of the time as possible and the performance of the system should be maintained at the highest possible level.

The Environmental Research Laboratory received the first quadrupole GC/MS/Computer system in the EPA four years ago. The maintenance techniques described in this report were compiled from experience gained during the past four years in the analysis of various types of organic pollutants (1, 2). When used in conjunction with the instrument instruction manual (3) and the software manual (4), these techniques have been effective in maintaining instrument stability and sensitivity.

Also, techniques were developed to simplify the interpretation of data. These include methods for acquiring better data and for extracting the maximum useful information from the data after it has been acquired.

SECTION III

EXPERIMENTAL

Gas chromatograph/mass spectrometer -- Results described were obtained using a Finnigan 1015-C quadrupole mass spectrometer interfaced to a modified Varian 1400 gas chromatograph by means of a glass jet separator.

Data system -- The data system was a System 150 supplied by System Industries and based on a Digital Equipment Corporation PDP-8e computer with 4K of core storage. I/O devices included a teletype, magnetic tape and magnetic disk data storage, x-y plotter, and mass spectrometer interface.

SECTION IV

RESULTS AND DISCUSSION

MAINTAINING MASS SPECTROMETER STABILITY

Instability in the mass spectrometer may cause drift that can invalidate the mass number calibration file used by the data system, leading to incorrect assignment of mass numbers. Interpretation of the resulting data is impossible. For example, in Figure 1, a spectrum of methyl linoleate, the molecular ion is shown at m/e 295 instead of at the correct value of 294. The calibration file used had been verified prior to data collection by obtaining spectra of the calibration standard and checking the accuracy of mass number assignment. In another case, a shift of less than one mass number was observed when a calibration with perfluorotributylamine (FC-43) was verified. The relative intensities of the mass 502 and 503 ions of the FC-43 spectrum were approximately equal instead of in the correct 10:1 ratio.

Checking for Drift

If the operator suspects that drift is occurring during a GC run, a check may be performed by taking several reference spectra at the end of the run. Just prior to the termination of data collection, FC-43 or any suitable standard may be introduced through the batch inlet system. The amount introduced should not produce a total ion current large enough to be the base spectrum in the RGC and it should not saturate the integrator. The standard spectra provide a simple means of checking for correct mass number assignment (Figure 2). Possible causes for this type of instability include heat, vacuum tube failure, and low temperature of the ionizer.

Heat

A common cause of instability is excess heat in the electronics of the mass spectrometer, particularly in the radio frequency generator chassis. This excess heat is usually caused by a dirty air filter or cooling fan failure. In an unusual case reported by Dr. D. Craig Shew of the Robert S. Kerr Environmental Research Laboratory, a change in component location by the manufacturer caused a power transformer to receive less cooling that it had received

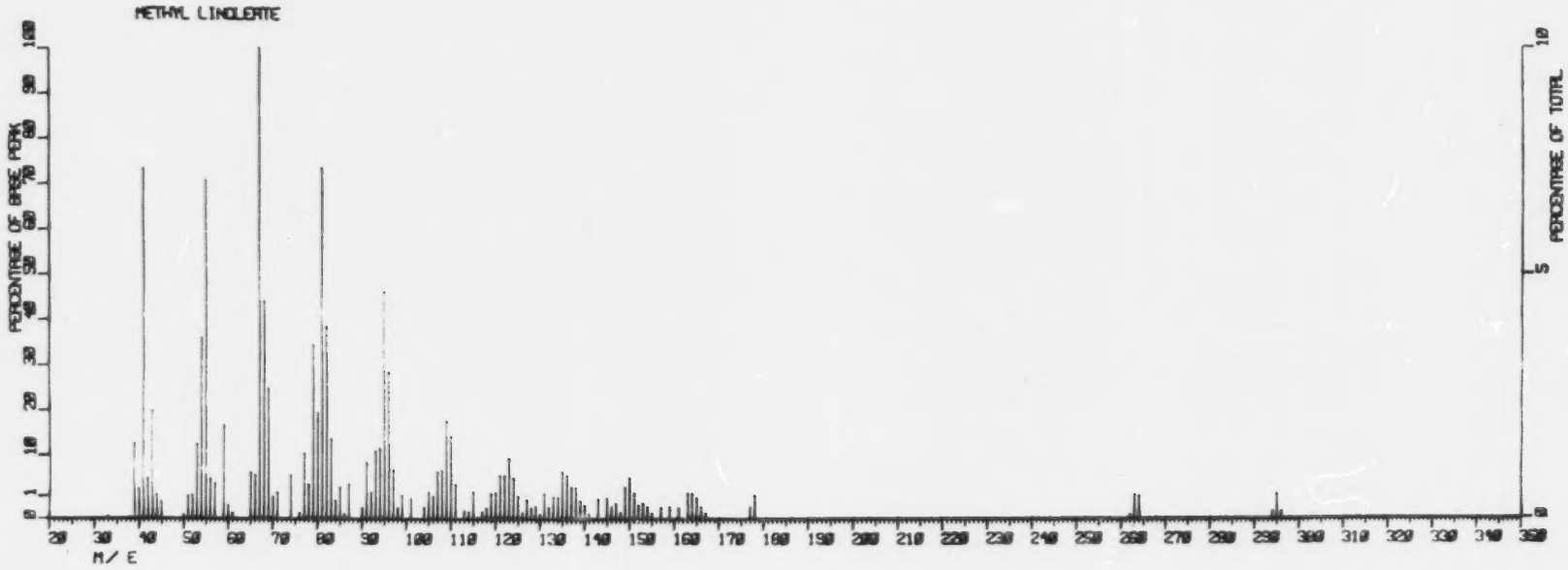

Figure 1. Spectrum of Methyl Linoleate Showing Incorrect Mass Assignment At m/e 295

previously. The resulting instability was corrected by boring holes in a chassis partition to increase air circulation to the transformer.

Vacuum Tube Failure

Drift is frequently caused by decline in vacuum tube performance. The three 807 tubes and the 6AL5 tube in the RF generator fail most frequently and may have to be replaced every six months. Instability in the reconstructed gas chromatogram (RGC) of FC-43 from the batch inlet system is an indication of tube failure.

Tube performance may be tested by introducing sufficient FC-43 (approximately 1 µl) to give an operating pressure of about 2×10^{-6} Torr with the separator blanked off. Integration times of 4 ms from mass 30 to mass 250 and 17 ms from mass 251 to mass 620 should be selected. In normal operation the amplitude of the total ion current for successive spectra varies by less than 5 percent. If the tubes are defective, the deviation in amplitude may be as much as 40 percent. After the tubes have been replaced and allowed to stabilize for at least an hour, the DC Zero and Balance procedure and the DC/RF Generator adjustment must be performed as described in the 1015 Instruction Manual.

Warmup Time

After the ionizer has been on for about fifteen minutes, a discrete shift in calibration may occur. According to Finnigan personnel, the shift may be caused by a change in quadrupole rod geometry induced by heat from the filament of the ionizer. The problem can be eliminated by turning the ionizer on for at least fifteen minutes prior to obtaining a calibration file on the data system. This is necessary mainly for GC runs longer than fifteen minutes.

MAXIMIZING SENSITIVITY

Lack of sensitivity in the mass spectrometer leads to higher noise levels because increased signal amplification is required. Furthermore, because of low sensitivity the need for large amounts of sample may preclude analysis of materials present at very low concentrations. It is therefore important to have maximum sensitivity available at all times.

Resolution adjustment must be performed daily to maximize mass spectrometer sensitivity. Appendix I outlines the adjustment procedure used regularly in our laboratory.

Periodic maintainance is also important in maintaining mass spectrometer sensitivity. We use a modified version of the Finnigan procedures in the Instruction Manual for the 1015-C for cleaning the quadrupole rods and the electron multiplier.

Quadrupole Rod Cleaning

The procedure recommended in the Finnigan manual was found to be insufficient when, following an instrument shutdown, a rapid loss of sensitivity and a drastic decline in peak shape quality was noted after the ionizer was turned on. The erratic behavior was found to be caused by a film on the rods, which was not removed by the suggested cleaning procedure. Therefore, a procedure was developed to remove the deposit. After removing the black dielectric deposits from near the ends of the rods by rubbing with an alumina-methanol slurry and a cotton-tipped swab, the rods were cleaned with successive washes of ethyl acetate, acetone, and methanol. This multi-solvent washing was found to be more effective for the removal of organic films than a rinse with methanol alone.

Electron Multiplier Regeneration

A similar film on the electron multiplier inhibited regeneration. The multiplier was cleaned with successive washes of the three solvents mentioned previously, and it was baked in air for one hour at 340°C. After baking, the multiplier was reinstalled and placed under vacuum as quickly as possible to prevent degeneration by atmospheric water vapor. This procedure resulted in a five-fold increase in sensitivity. The multiplier has been regenerated eight times with no overall decline in performance.

Separator Clogging

The separator also has a significant effect on the sensitivity of the GC/MS system. If the separator is partially clogged or the carrier gas flow is adjusted improperly, sensitivity is markedly reduced. A partially clogged separator is indicated when solvent peaks tail

excessively or the operating pressure of the system approaches the pressure of the system with the separator sealed off. If a clogged separator is suspected, the jets should be inspected for foreign matter with a small magnifying glass.

A minimum carrier gas flow of 14-16 ml per minute is required for satisfactory separator operation. Optimum efficiency may occur at an even higher flow rate, which can be used if GC resolution is not critical. Separator effects will be further discussed in the next section.

Solid Probe

A very simple method for increasing GC/MS sensitivity is the insertion of the solid sample probe into the ionizer. A clean sample container should be in place at the tip of the probe. Insertion of the probe results in a more tightly enclosed ionizing volume, which in turn provides a higher concentration of sample molecules for ionization (5). The temperature of the probe should be adjusted to approximately that of the instrument manifold.

SIMPLIFYING INTERPRETATION

One problem in the interpretation of GC/MS data is in the comparison of quadrupole with magnetic deflection mass spectra. Low mass ion intensities are enhanced by the quadrupole system, causing the relative intensities of high mass ions to be lower than those obtained on magnetic instruments. The tune-up procedure outlined in Appendix I is one technique to enhance high mass ion intensity.

Another way to achieve this enhancement is to make a judicious choice of spectra for output. By choosing a spectrum from the leading edge of the RGC peak, high mass relative ion intensity can be increased. On the leading edge of the RGC peak sample concentration is increasing during the scan and, since the 1015-C scans from low to high mass, more sample is in the ionizer during the high mass portion of the scan.

Figure 2 shows the RGC of a decafluorotriphenylphosphine sample supplied by the Analytical Quality Control Laboratory (AQCL), Cincinnati. Figure 3a is a spectrum from the leading edge of the RGC peak and Figure 3b is a spectrum from the trailing edge of the peak. The higher intensity of the M^+ ion at mass 442 is evident in Figure 3a. This effect

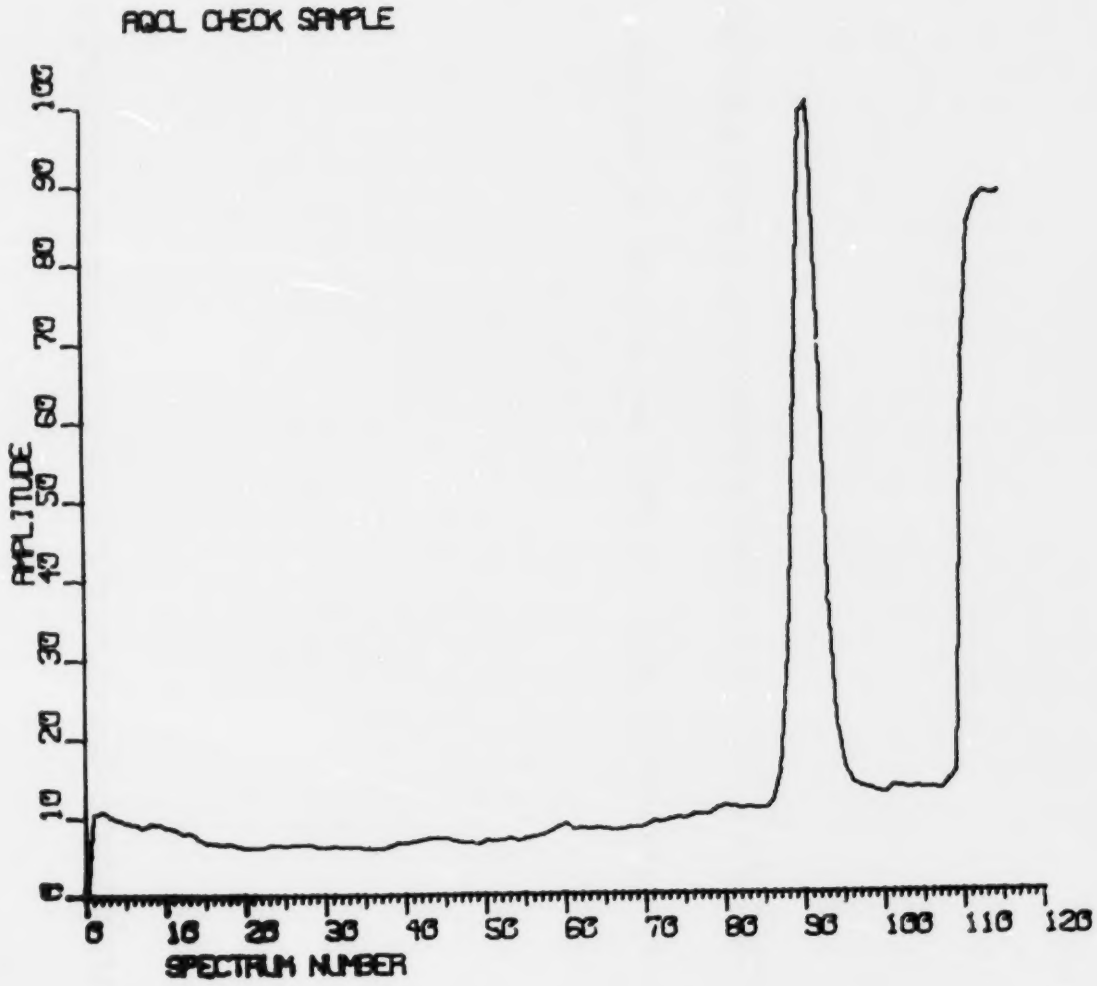

Figure 2. Reconstructed Gas Chromatogram of Decafluorotriphenylphosphine With FC-43 Reference at End of Run

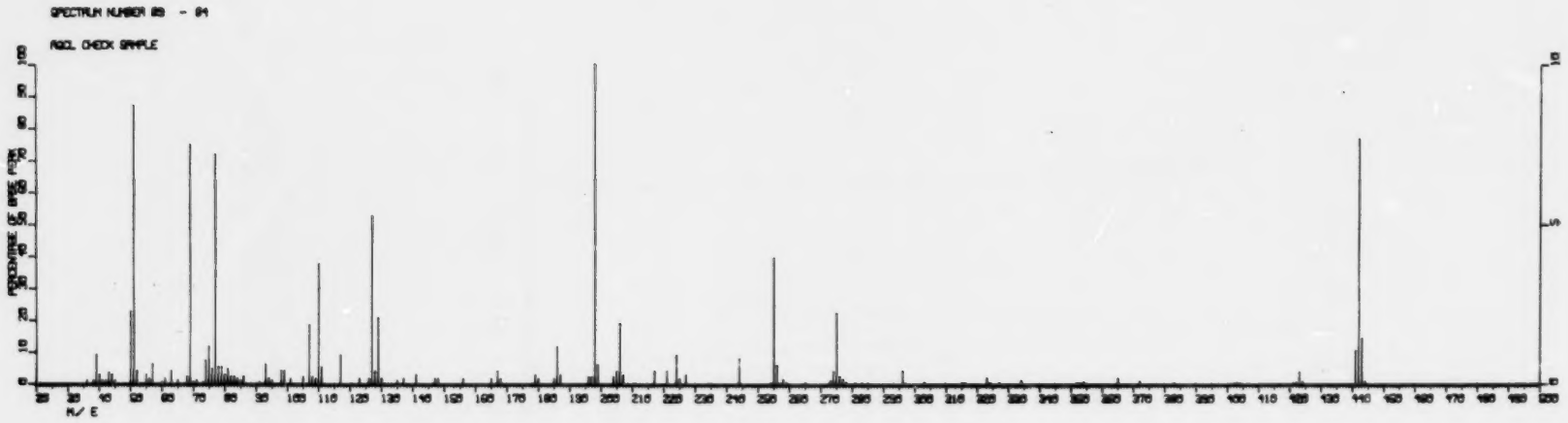

Figure 3a. Decafluorotriphenylphosphine Spectrum From Leading Edge of RGC Peak

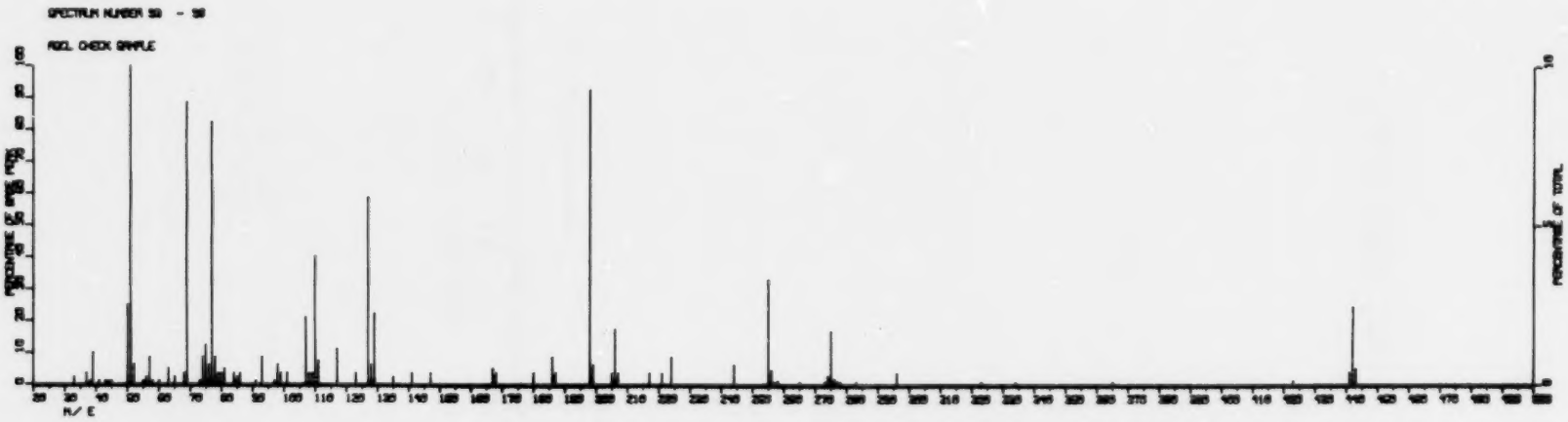

Figure 3b. Decafluorotriphenylphosphine Spectrum From Trailing Edge of RGC Peak

will be most pronounced when scan times are long with respect to GC elution times.

Correlating Gas Chromatograms

Another problem encountered was a difficulty in correlating GC/MS RGC's with gas chromatograph runs made on the same 50' SCOT column in an off-line GC operated with a flame ionization detector at atmospheric pressure. The column appeared to have greater efficiency when it was connected in the GC/MS. This problem was solved by adjusting the carrier gas flow of the off-line GC to approximately one half the flow through the GC/MS. The flow rate through the GC/MS was measured before the column was connected to the separator and was checked after connection by measuring the exhaust from the separator vacuum pump.

The higher efficiency on the GC/MS column may result from a higher pressure at the column outlet caused by the constriction in the jet separator. The inlet pressure was the same in both instances. According to McNair and Bonelli (6), column efficiency is increased as the ratio of inlet to outlet pressure approaches unity.

Optimum Integration Time

A technique for obtaining good spectra from low sample concentrations is the use of the longest integration times that are practical from the standpoint of peak elution times and integrator saturation. In the System 150 software, the analog to digital converter (ADC) value for each mass is normalized to 1 ms integration time by dividing it by the integration time for that mass. Normalization of the small ADC values obtained with short integration times and small amounts of sample, however, results in many masses having the same amplitude, as illustrated in Figure 4 from mass 33 to 250.

Figure 4 is the mass spectrum of a compound found in the effluent of a pesticide manufacturing plant and tentatively identified as nonachlor. The integration time from mass 33 to 250 was set at 2 ms because of some large GC peaks in the sample. The integration time from mass 251 to 450 was 17 ms. The data above mass 250 show better statistical quality because of the longer integration time.

We usually try to compensate for the lower sensitivity of the quadrupole at high mass by using longer integration

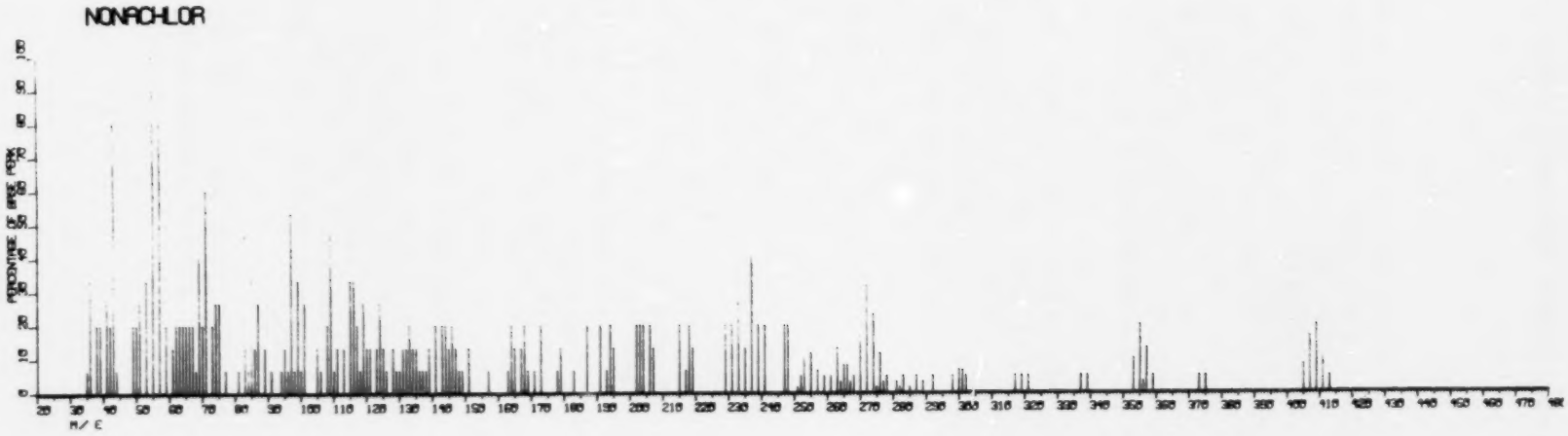

Figure 4. Spectrum of Nonachlor Obtained Using 2 ms Integration Time Below Mass 250 and 17 ms Integration Time Above Mass 250

times for masses above 250. A typical choice of integration times and mass ranges in the high mass range is 4 ms from mass 33 to 250 and 17 ms above mass 250.

The signal optimization mode of data collection or IFSS (Integration time as a Function of Signal Strength) can give better data on small RGC peaks while not saturating on large peaks. However, since the instrument integrates longer on small peaks than large ones, some spectra take longer than others and the Spectrum Number scale of the RGC is not linear with respect to time. The RGC will therefore be distorted when compared to a GC run. The IFSS mode has been found to use more disc or tape storage than the normal, or CONTROL, mode.

Superimposed LMRGC's

The utility of limited mass range reconstructed gas chromatograms (LMRGC's) can be increased by superimposing LMRGC's on RGC's or other LMRGC's. One application of this technique is in the analysis of unresolved GC peaks, as illustrated in Figure 5, the RGC of a paper mill effluent. The major GC peak at spectrum number 127 appears to be due to a single component. However, two terpenes likely to be in this sample were known to have practically identical retention times on the column being used. The terpenes were alpha-terpineol, which has a base peak at mass 59, and borneol, which has a base peak at mass 95. Therefore two LMRGC's, one for mass 59 and one for mass 95 were superimposed, as shown in Figure 6.

Based on the information obtained from the superimposed LMRGC's, two background-subtracted spectra were plotted. The plot of spectrum 124-123 is shown in Figure 7 and spectrum 130 minus spectrum 124 multiplied by an amplification factor of 0.5 is shown in Figure 8. These two spectra indicated that both components were present in the sample. The result of matching these spectra on the Battelle/Biemann matching program is shown in Figure 9. A similarity index (SI) of 1.00 is a perfect match.

Superimposed LMRGC's can also be used to indicate classes of compounds. Figure 10a is the RGC of a methylated paper mill effluent sample. The two main peaks in the mass spectra of methyl esters of saturated fatty acids are at masses 74 and 87. Methyl esters of fatty acids are indicated by simultaneous peaks on both LMRGC's, such as at spectrum number 255 of Figure 10b. Mass spectrum 255 was that of methyl palmitate.

Appendix II gives a procedure for superimposing RGC's and LMRGC's. This procedure, furnished by Mr. J. G. Watt of System Industries, eliminates redrawing the axes of the graph with each successive plot.

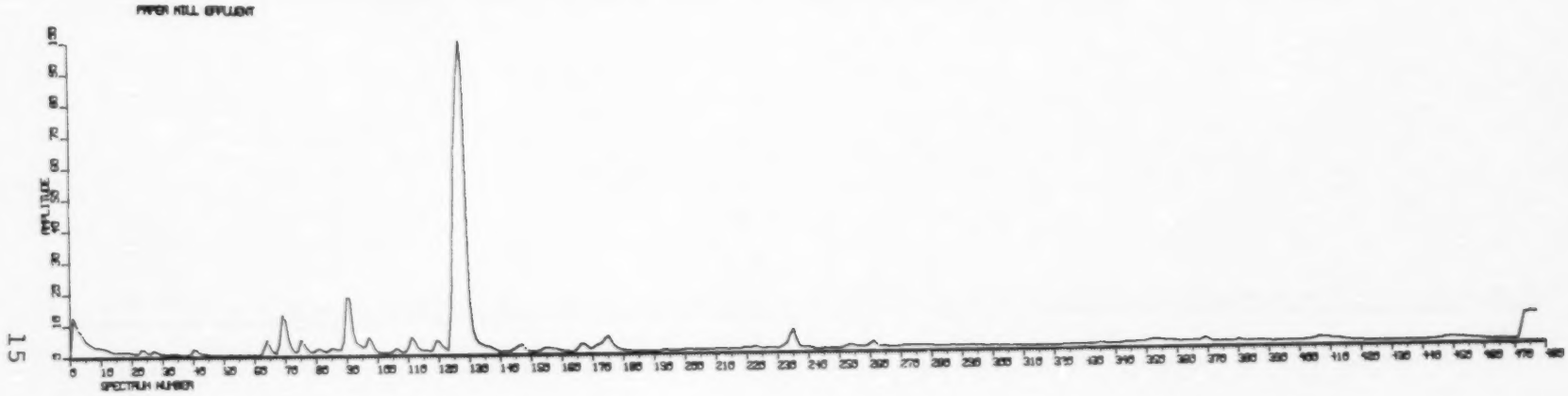

Figure 5. Reconstructed Gas Chromatogram of Paper Mill Effluent

Figure 6. Superimposed Mass 59 and Mass 95 Limited Mass Range Reconstructed Gas Chromatograms of Paper Mill Effluent

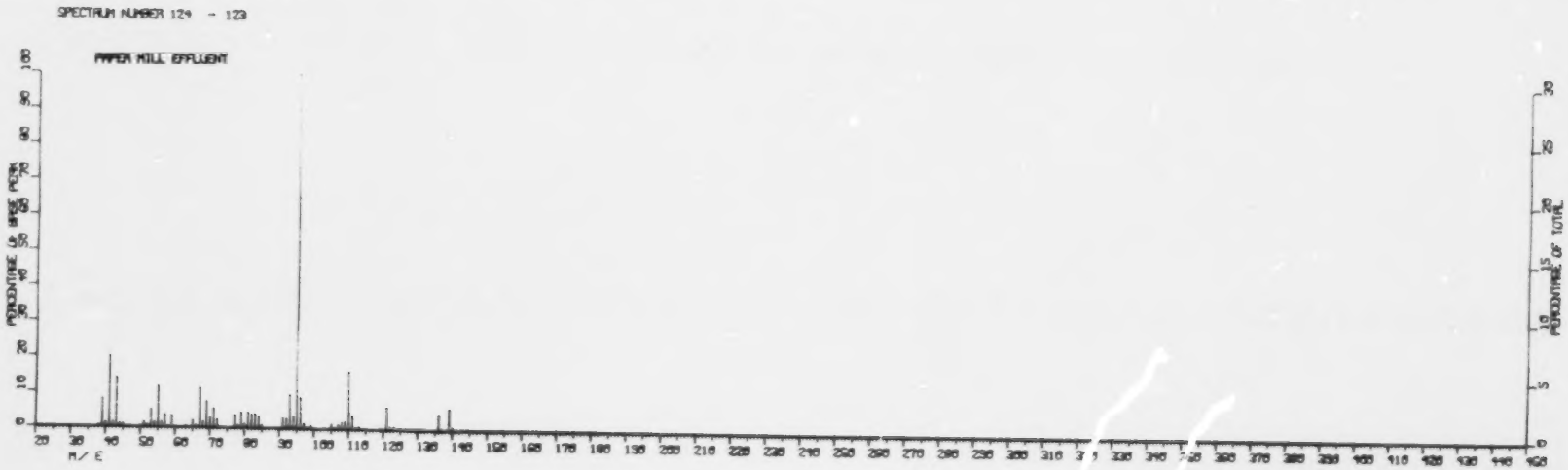

Figure 7. Spectrum 124 Minus 123 of Paper Mill Effluent (Borneol)

Figure 8. Spectrum 130 Minus 124 multiplied by 0.5 of Paper Mill Effluent (Alpha-Terpineol)

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S, E, P, R, OR C? S
I.D.?  PAPER MILL SAMPLE
PAPER TAPE?N
FN--I1T124; SP--1
PAPER MILL EFFLUENT
PARMTRS?      M9Ø-2ØØ
45 HITS
BORNEOL (SEWL)↑L55 ATJ A A B CG↑ 154 C1Ø.H18.0 BSR Ø212
FILE KEY=  8697
SI=Ø.811

ISOBORNEOL (SEWL)↑L55 ATJ A A B CO↑ 154 C1Ø.H18.Ø BSR Ø215
FILE KEY=  8700
SI=Ø.7Ø6

2,5- DIMETHYL 2,4-HEXADIENE 11Ø C8.H14 AST ØØ2Ø
FILE KEY=     17
SI=Ø.392

ISO-BORNEOL 154 C1Ø.H18.0 MSC 1711
FILE KEY=   6296
SI=Ø.363

2,3-DIMETHYLHEXA-1,4-DIENE 11Ø C8.H14 MSC 3265
FILE KEY=   78Ø7
SI=Ø.351

S, E, P, R, OR C?S
I.D.?  PAPER MILL SAMPLE
PAPER TAPE?N
FN--I1T130;SN--1;:
PAPER MILL EFFLUENT

PARMTRS?          M100-350
 59 HITS
ALPHA-TERPINEØL 154 C10.H18.Ø MSC 1720
FILE KEY=  6305
SI=0.717

2-TERPINEØL 154 C10.H18.Ø AST 1671
FILE KEY=  1133
SI=0.682

MYRCENØL (SEWL) 152 C10.H16.Ø BSR 0210
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Figure 9. Computer Matches of Spectra in Figures 7 and 8

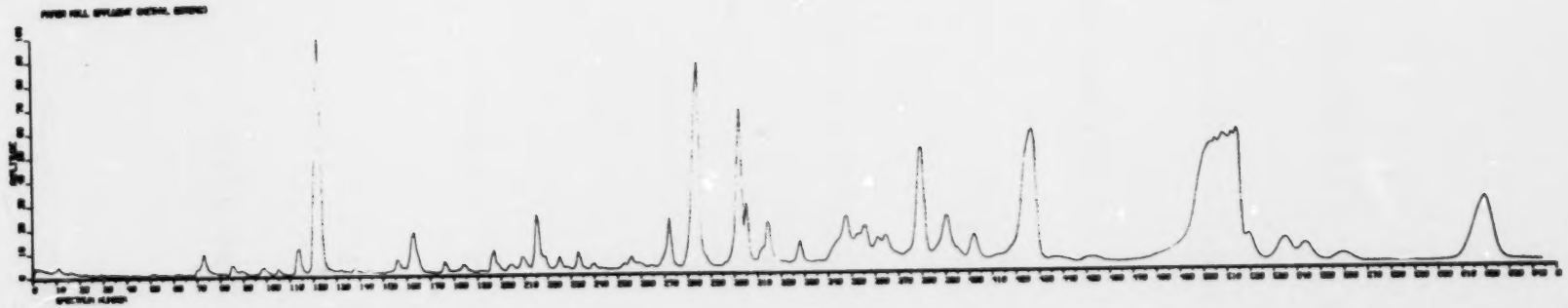

Figure 10a. Reconstructed Gas Chromatogram of Paper Mill Effluent (Methyl Esters)

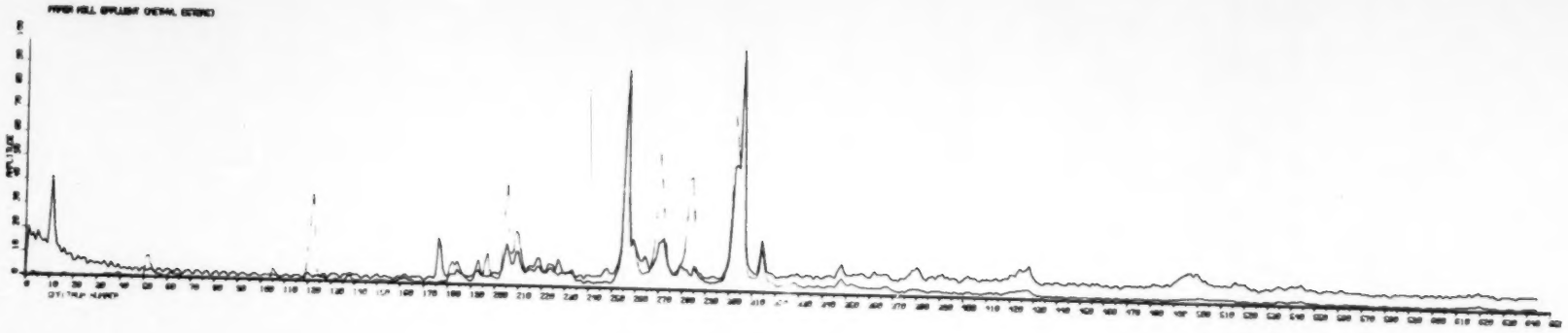

Figure 10b. Superimposed Mass 74 and Mass 87 Limited Mass Range Reconstructed Gas Chromatograms of Paper Mill Effluent (Methyl Esters)

SECTION V

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SECTION VI

GLOSSARY

FC-43 -- perfluorotributylamine, a calibration standard material.

GC -- gas chromatography, a separation technique based on the partition of materials between gas and liquid phases.

GC/MS -- a union of GC and MS in which the chromatograph effluent passes precludes a separator into a mass spectrometer inlet.

LMRGC -- limited mass reconstructed gas chromatogram, a computer output that shows the relative currents resulting from positive ions of particular mass-to-charge ratio reaching the mass spectrometer detector as a function of scan number.

M^+ -- the ionized molecule, produced by the removal of one electron with no accompanying fragmentation of the ion.

MS -- mass spectrometry, an identification technique based on the fragmentation of ionized materials.

RGC -- reconstructed gas chromatogram, a computer output that shows the relative currents resulting from summing all positive ions reaching the mass spectrometer detector as a function of scan number. This plot usually resembles the chromatogram obtained in GC.

APPENDIX I

Resolution Adjustment Procedure

We use the following procedure to adjust the high mass range resolution on our Finnigan 1015-C. This is a modification of the procedure outlined on pp 6-15 through 6-19 of the 1971 1015-C manual.

The data system should be in the MANUAL mode of operation so that spectra are displayed on the oscilloscope. Sufficient FC-43 should be introduced through the batch inlet to give an amplitude at mass 502 of at least 3 cm at a scope sensitivity of 20 mV/cm.

The ion energy is set to 5V. The peak at mass 264 should be maximized by adjusting the extractor voltage and the lens voltage. Next, resolution between masses 69 and 70 is adjusted to baseline resolution (Figure 11a) with trimpot R-81 on circuit board PC.5. Resolution between masses 219 and 220 is then adjusted to a valley of approximately 50% of mass 220 amplitude (Figure 11b) with trimpot R-77. Since the adjustments of R-81 and R-77 interact, the two adjustments should be repeated until the desired resolution at both points is achieved. After accomplishing this, the resolution between masses 502 and 503 is adjusted to a valley of approximately 90% of mass 503 amplitude with trimpot R-180 (Figure 11c).

The high mass range of the 1015-C has a secondary amplifier circuit to enhance high mass intensity. The lower mass threshold of this circuit is set by the following procedure. The same oscilloscope display of the FC-43 spectrum as mentioned previously is used.

The first and last mass controls are set so that the mass 219 peak is at the left side and the mass 264 peak is at the right side of the oscilloscope display. Then, the amplifier gain of the circuit is set to maximum by turning trimpot R-180 fully counterclockwise. Next, trimpot R-179 is adjusted to give a baseline rise approximately one cm to the left of mass 264. Finally, R-180 should be readjusted to give the desired resolution between masses 502 and 503.

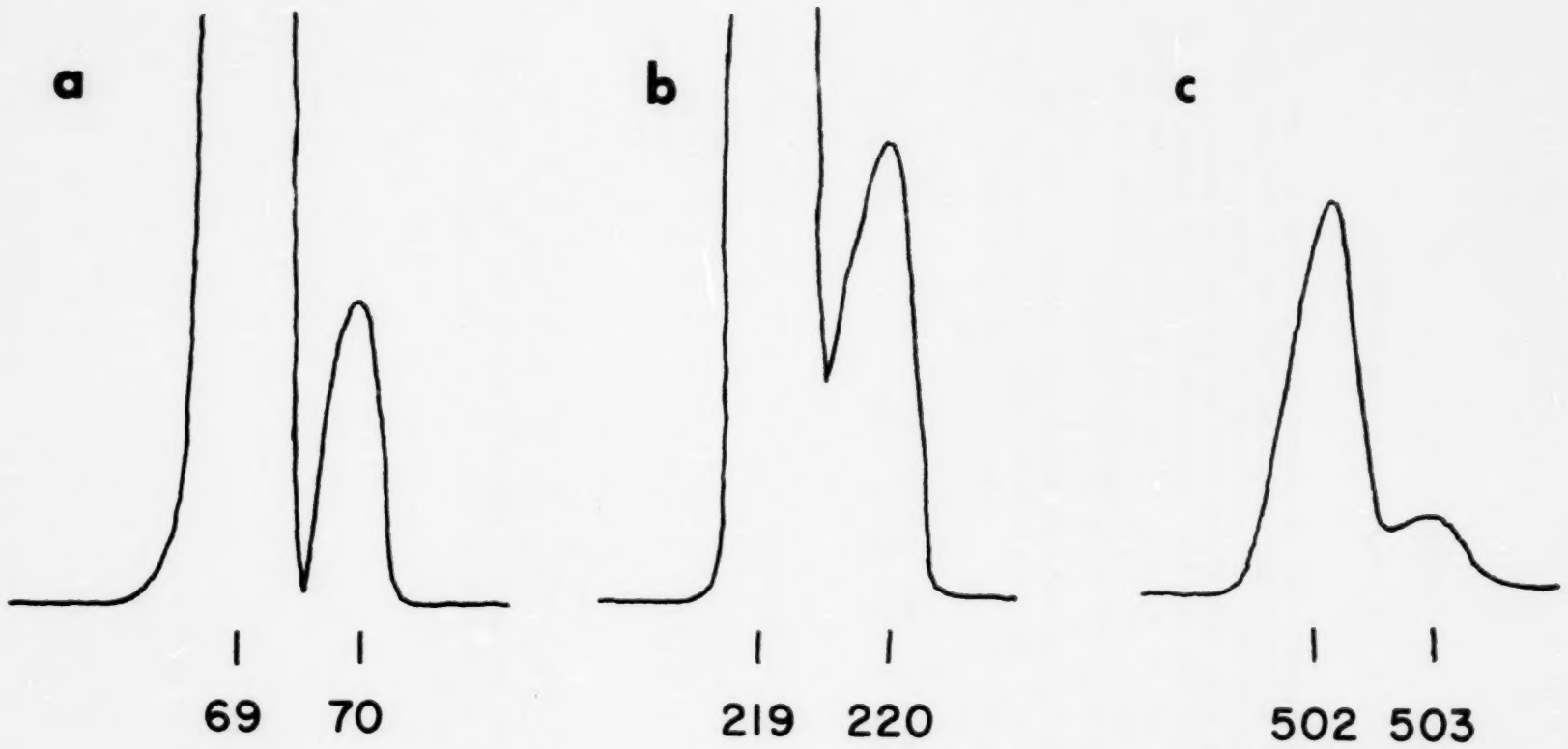

Figure 11 a. Baseline Resolution Between Masses 69 and 70
b. 50% Valley Resolution Between Masses 219 and 220
c. 90% Valley Resolution Between Masses 502 and 503

APPENDIX II

Procedure for Superimposing LMRGC's

The procedure to bypass the construction of axes by the plotter involves halting the computer, making 3 changes in the memory of the PDP-8, and restarting the computer. The first step is to plot the first RGC or LMRGC, including axes. Then, enter the output parameters for the LMRGC to be superimposed on the original. After responding to the final prompt, "EXPAND BY:", wait until the plotter begins to move and stop the computer with the "HALT" switch.

At this point, manually relocate the pen position to the origin of the axes. This should be done with care so that the spectrum mumbers of the traces will correspond. A different color pen, which further simplifies interpretation, can be inserted at this point. The following changes then must be toggled into the memory of the PDP-8 by means of the switch register. All numbers are octal.

Location	Old Instruction	New Instruction
2007	4731	7000 (NOP)
2010	4732	7000 (NOP)
2013	1737	5271 (JMP Begin Trace)

Finally, the starting address of 1777 is loaded into the switch register and the "LOAD ADDRESS", "CLEAR", and "CONTINUE" key are pressed. After a brief (in the case of the disk system) pause the plotter will superimpose the LMRGC on the original axes.